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14. ABSTRACT

Polyurea is a microphase-separated block copolymer that has been shown to effectively mitigate blast-induced failure of steel and other structural materials. Polyurea exhibits unique properties, including pressure-dependent compressive stiffness, low tensile stiffness, high dissipation, and residual stiffness at high deformation levels, as a result of its morphology. These and other mechanical and physical attributes of block copolymers can be greatly enhanced and specifically tailored to manage stress waves over multi-frequency ranges. The technical objectives of the ONR-BRC are (1) to develop rules and tools for the creation of elastomer-based composites that can mitigate shocks and stress pulses over broad ranges of frequency and amplitude and (2) to optimize their compositions and characteristics at molecular/nano-, micro-, meso- and macro-scales. An integrated approach was used to address the fabrication, modeling, and characterization needs; involving integration of • Numerical and analytical design• Chemical synthesis, • Elastomer-based composites, and • Characterization and validation

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Final Technical Performance Report

ONR Grant Number: N00014-09-1-1126

Grant Title: Elastomeric Polymer-by-Design for Blast-Induced Shock-Wave Management

PI: Sia Nemat-Nasser, UC San Diego

Performance Period: September 30, 2009 - November 30, 2014

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ABSTRACT [Status of Effort]

Polyurea is a microphase-separated block copolymer that has been shown to effectively mitigate blast-induced failure of steel and other structural materials. Polyurea exhibits unique properties, including pressure-dependent compressive stiffness, low tensile stiffness, high dissipation, and residual stiffness at high deformation levels, as a result of its morphology. These and other mechanical and physical attributes of block copolymers can be greatly enhanced and specifically tailored to manage stress waves over multi-frequency ranges.

The technical objectives of the ONR-BRC on Elastomeric Polymer-by-Design for Blast-Induced Shock-Wave Management are (1) to develop rules and tools for the creation of elastomer-based composites that can mitigate shocks and stress pulses over broad ranges of frequency and amplitude and (2) to optimize their compositions and characteristics at molecular/nano-, micro-, meso- and macro-scales.

An integrated approach was used to address the fabrication, modeling, and characterization needs. Hybrid polymer grafted nanoparticles for reinforcing polyurea, and superlattice nanocomposites were developed. Chemical and geometrical parameters were studied for their influence on the thermomechanical properties of the resulting materials. The effect of surface treatment on micron-scale milled glass fiber-reinforced polyurea composites was studied. Chemical effects of changing stoichiometry, introducing blowing agents to control porosity, and environmental aging were addressed. Thermomechanical data for various cases were used to develop constitutive parameters and master curves for FEM codes. Modeling has been performed at three length scales: nano-, meso-, and macro-/continuum. The chemical structure was modeled at nano-scale via all-atom simulations to determine coarse-grained properties. The coarse-grained parameters were then used to model the chain dynamics of polyurea under realistic shock conditions and to predict their thermomechanical constitutive properties. Continuum scale models and homogenization techniques were utilized to establish the overall response of composites.

Lastly, to supplement the aforementioned research efforts, we also developed an innovative experimental technique as well as the corresponding computational simulations to characterize polyurea at extreme conditions. An experimental facility was designed and constructed to subject polyurea to combined high pressure and shear at high strain rates, and a finite element model was concurrently developed.

PROGRESS STATEMENT

Our efforts in the final phase of the ONR-BRC program have focused on understanding polyurea in extreme conditions and are summarized here in two primary thrusts: experimental and computational efforts.

First, our work on the design and development of innovative experimental techniques to achieve extreme pressures and the resulting characterization is reported. This includes our work spanning a wide pressure range including ambient, mild, high and very high pressures. For the ambient pressure regime, we conducted ultrasonic measurements, dynamic mechanical analysis (DMA), and differential scanning calorimetry (DSC). For the mild pressure regime (up to 10 MPa), we designed compressive-mode confinement cells to use in combination with ultrasonic wave measurement techniques. We also designed a second compressive-mode confinement cell for high pressure (up to 1 GPa). Additionally, we developed a 1" gas gun to fire a ½" steel ball projectile at a polyurea sample to create impact-induced high rate shearing under high pressure. Finally, for the very high-pressure regime (0.5 – 20 GPa) we are using a diamond anvil cell combined with optical spectroscopy to observe the behavior of polyurea at extreme pressure.

Second, our work on the modeling efforts, which is divided into three length scales (nanoscale, mesoscale, and macro/continuum scale), is reported. At the nanoscale, molecular dynamics (MD) simulations have been performed with the accurate COMPASS potential for representative volumes of short oligomer polymer chains. The structural distributions of polyurea extracted from these simulations were then used to calibrate a coarse-grained (CG) model of polyurea using the Iterative Boltzmann Inversion (IBI) method. From equilibrium simulation of these CG models we have calculated the stress relaxation function of a linear polyurea with realistic molecular weights from which the frequency dependent storage and loss moduli can be computed. The predictions from these molecular simulations shed light on the dissipative properties of polyurea as well as elucidate trends in key chemical structure-property relationships. Additional coarse-grained models were created to study the effect of nano-inclusions with grafted polymer chains on the stress relaxation in polymer nanocomposites. At the continuum scale, the extended finite element method (XFEM) has been adapted to study the dissipative properties of inclusions within a polymer matrix. Furthermore, by considering interfaces that can fail in tension or shear loading, the feasibility of designing weak interfaces to further enhance energy dissipation has been studied.

Experimental Efforts

Impact-Induced High Rate Shearing under High Pressure: Experimental Technique

We have designed and constructed an experimental facility (Figure 1) to subject polyurea to combined high pressure and shear at high strain rates. A 1" gas gun fires a ½" steel ball bearing projectile using a polymer foam (modulan) sabot. At the end of the barrel, the velocity of the sabot and projectile are recorded, and sabot it stripped away. The projectile continues towards the target, and its velocity is measured a second time. The target is a flat 1 mm thick layer of polyurea positioned over a premade dimple on a ½" diameter steel bar. The projectile pushes the polyurea into the dimple, creating local regions of combined high pressure and shear in the sample. The incident velocity of the ball bearing is chosen to damage the polyurea, but not completely punch through it. Tests have been performed both with and without lateral confinement of the polyurea disc. The steel bar is instrumented with strain gages that record passing elastic waves from the impact, which can be compared with finite element analyses. The rebound velocity of the ball is measured, allowing the change in its kinetic energy to be estimated.

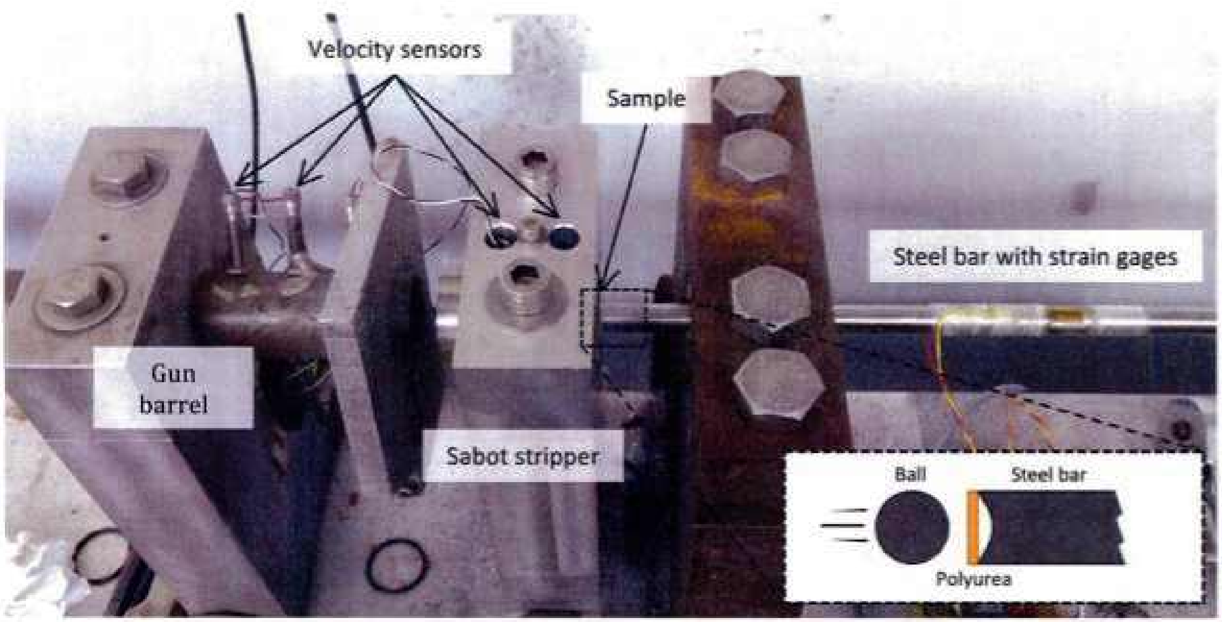

Figure 1: The experimental setup for producing combined high pressure and shear in polymer samples. The incident ball bearing exits the gas gun barrel (left), passes through a sabot stripper (center left), and impacts the polyurea sample (center) sitting at the end of a steel bar (right).

After testing, the impacted polyurea samples are studied in a postmortem analysis. Visual inspections of the samples typically show a slightly off-center biconcave region where the polyurea is thinner than the surrounding material (Figure 2). Outside of this region, streaks and spots of material radiate outward and resemble a splash pattern. Inside the region, there are bubbles in the material that were not present before testing. Our current hypothesis is that these bubbles are the result of depolymerization due to high temperatures and the isocyanate trying to evaporate. Finite element models of the test indicate rapid heating of the sample during impact, with localized regions reaching approximately 200 °C. When we place a virgin sample in a preheated 200 °C oven, it softens significantly and numerous bubbles form and grow (Figure 3 insert). A subsequent IR test of this rapidly heated material shows a loss of the peak associated with the urea linkage (Figure 3). DSC tests of the biconcave region in the impacted sample show a large, broad endothermic peak in the heat flow centered around 90 °C that initially disappears after heating, but reappears over after a day or more at room temperature. This suggests the presence of a crystalline or semi-crystalline structure, which could be trapped depolymerized isocyanates.

Figure 2: A ½" diameter polyurea sample after impact testing viewed at different optical zoom levels (increasing left to right).

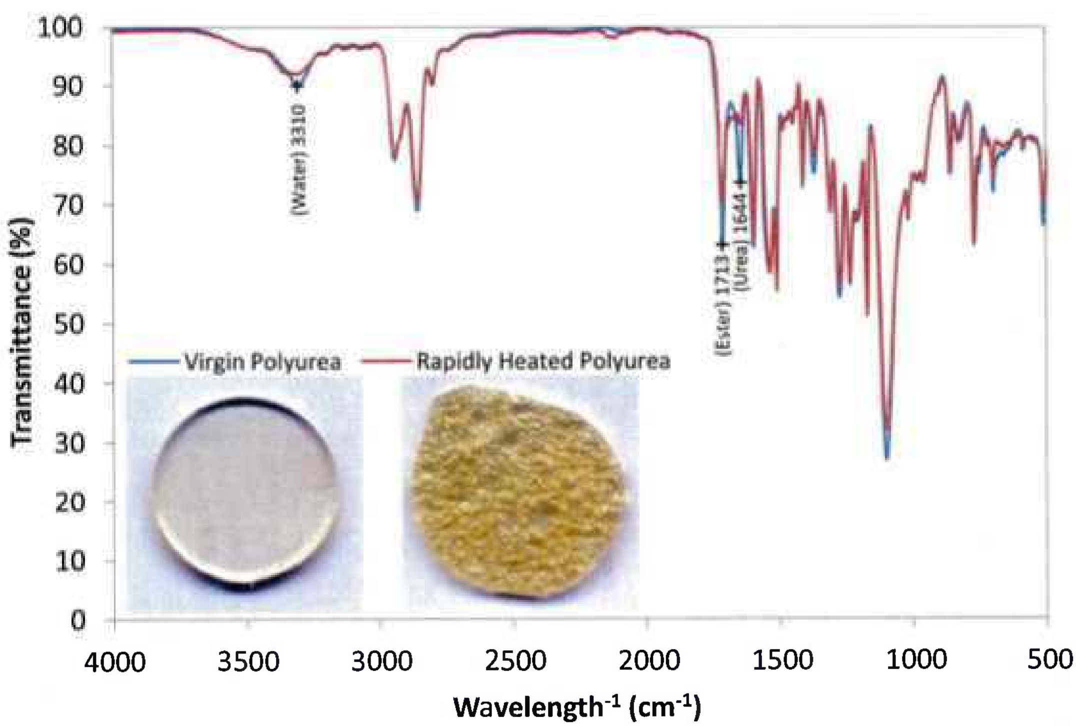

Figure 3: IR spectroscopy results for virgin polyurea and polyurea that had been rapidly heated in a 200°C oven.

It was noted that slowly heating polyurea to 200 °C over a period of an hour did not result in bubbles. It could be that the slow heating allows the isocyanate time to diffuse out of the sample or react to form other thermally stable structures. The mechanical properties have still changed significantly however as indicated by the master curves developed from DMA bending measurements (Figure 4). We have also measured the weight of polyurea before and after heating. 0.81% weight loss is observed due to the slow heating, and 0.73% due to the fast heating.

For another variant of polyurea, which is fabricated using Versalink P-650, similar permanent changes are observed. The weight loss due to the fast heating is 0.84%, and the weight loss due to the slow heating is 1.0%. Bubbles or cracks are formed in the fast heating, while the sample stays intact in the slow heating. Similar to PU-P1000, the mechanical properties have changed significantly after the slow heating process (Figure 4).

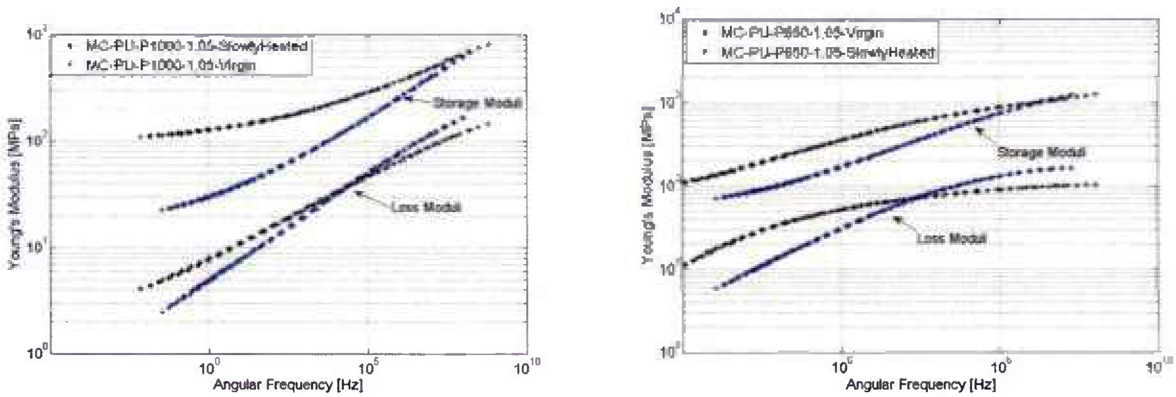

Figure 4: Master curves of pure polyurea PU-P1000 (left) and PU-P650 (right) at reference temperature 0°C for the virgin case and after being slowly headed to 200°C and then cooled to room temperature.

Ultrasonic Measurements at Mild Pressure and High Pressure

We have developed experimental techniques to measure the material properties of polyurea under various extreme conditions. Recently, we have focused high frequency testing at both mild pressure (up to 10 MPa) and high pressure (up to 1 GPa) levels. Compressive-mode confinement cells for the two pressure regimes have been fabricated (see Figure 5). Using the confinement cells coupled with ultrasonic wave measurement techniques, we are able to study the response of polyurea under extreme conditions.

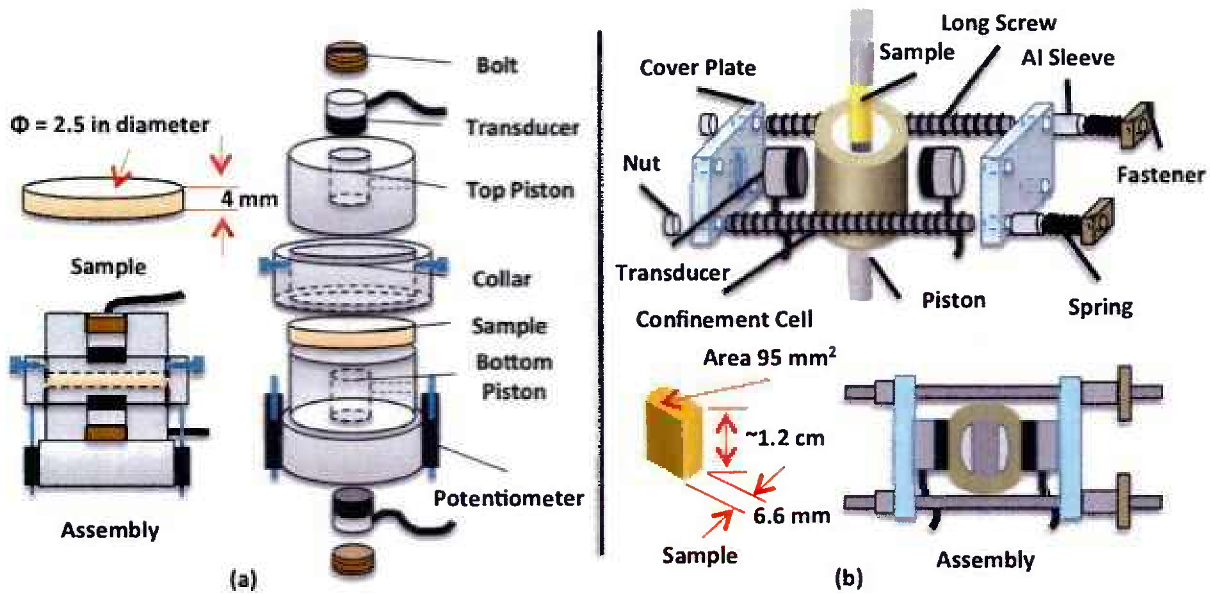

Figure 5: Compressive-mode confinement cells for (a) mild pressure up to 10 MPa and (b) high pressure up to 1 GPa.

We have completed testing studying the effect of pressure and frequency on longitudinal modulus of polyurea. The results that we obtained together with DMA master curve data of polyurea allows us to create a shift factor surface as a function of pressure and temperature (see Figure 6). With the shift factor surface, the complete master curve of polyurea can be obtained, allowing one to find the Young's storage and loss moduli at any desired temperature, pressure, and frequency.

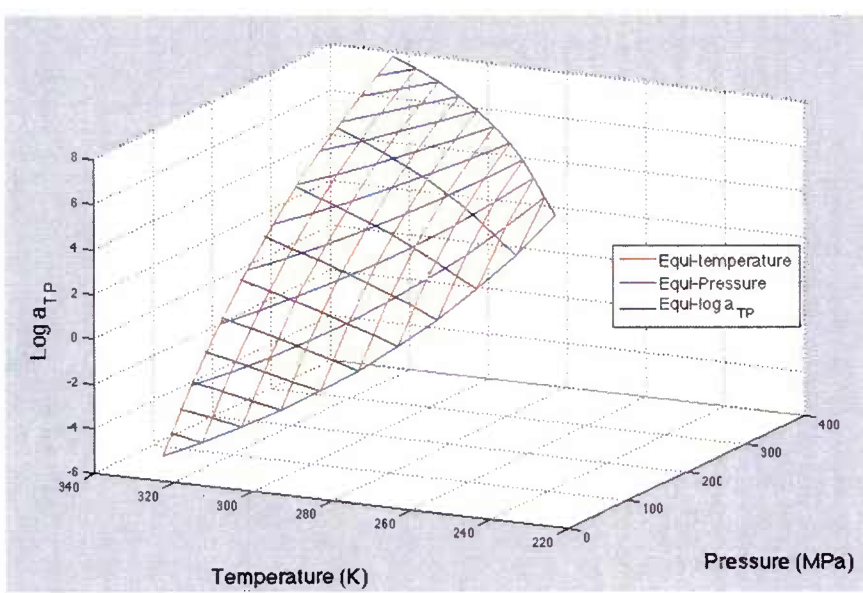

Figure 6: Shift factor surface for polyurea as a function of temperature and pressure at 273 K reference temperature and 1 atm reference pressure.

Diamond Anvil Cell: Very High Pressure

To observe the behavior of polyurea under very high-pressure over 3 GPa, first a pure polyurea sample (306 x 290 x 60 µm) was prepared. The sample was then placed in the hole of a gasket (340 x 330 x 100 µm), sitting on the lower diamond flat belonging to the cylinder side followed by putting two ruby spheres (2 µm diameter) as pressure sensors. As soon as filling the hole with 4:1 mixture of methanol:enthanol as a pressure transmitting medium, the gasket hole was sealed by bringing the piston anvil onto it.

In general, pressure is generated in a diamond anvil cell (DAC) by tightening the three or four symmetrically located screws. The DAC at UCSD/CEAM uses four symmetrically located screws. In this test, however, only two screws of them were tightened to generate pressure in order to apply pressure asymmetrically. As a result, we found that the circular gasket hole became elliptically deformed.

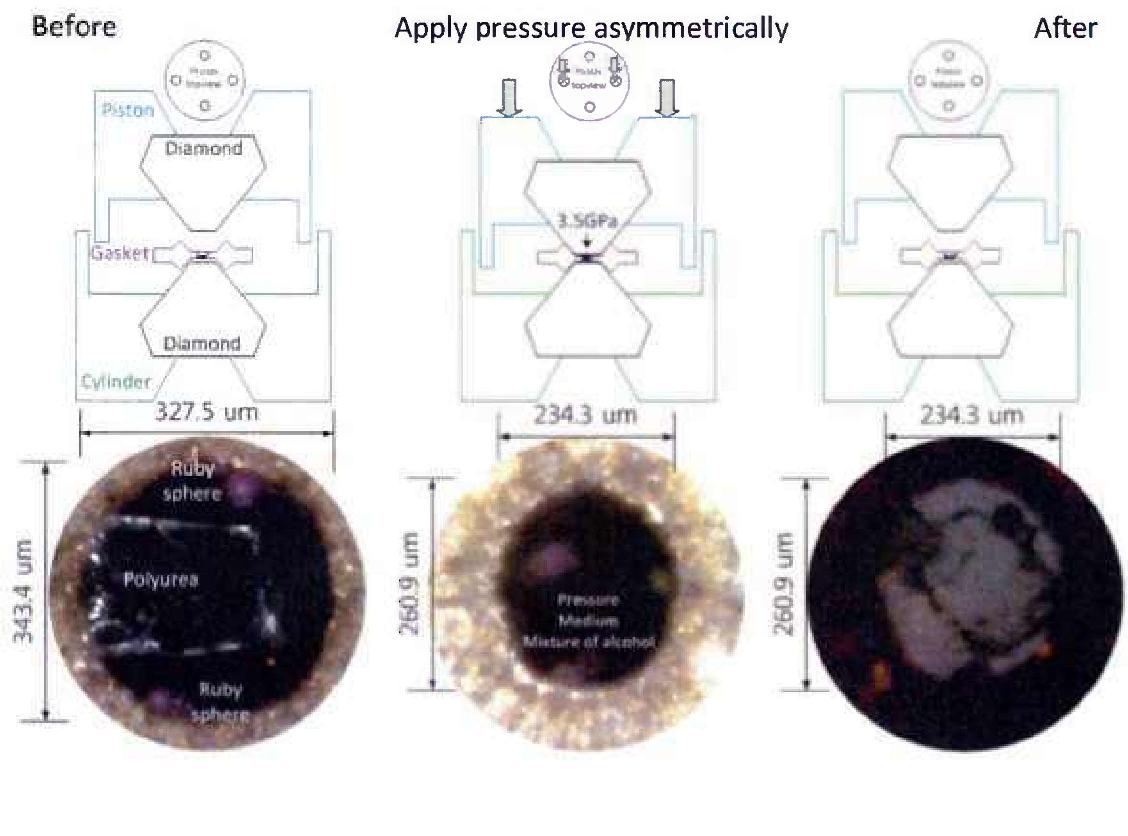

Figure 7: Diamond anvil gasket with asymmetrically applied pressure.

While the initial studies were interested in the shape change of materials under high pressure, our focus has shifted to studying the change in mechanical properties of polyurea with hybrid polymer grafted nanoparticles under very high pressure using the DAC. Eighteen parametric variations of polyurea with hybrid polymer grafted nanoparticle were prepared with different chain length, chain density, particle size, and silica weight percent. The sample size (approximately 100 x 100 x 50 μm) for the DAC experiments is limited by the size of the sample hole in a cell gasket. Therefore, an atomic force microscopy (AFM) with a sharp tip of less than 10 nm in diameter at the apex has been used to find the Young's modulus of the materials. The polyurea with hybrid nanoparticle samples subjected to a very high-pressure environment will be investigated and compared with control samples to determine the very high-pressure effect.

Computational Efforts

The modeling efforts are divided into three length scales (nanoscale, mesoscale, and macro/continuum scale) as illustrated in Figure 8. At the nanoscale, molecular dynamics (MD) simulations have been performed with the accurate COMPASS potential for representative volumes of short oligomer polymer chains. The structural distributions of polyurea extracted from these simulations were then used to calibrate a coarse-grained (CG) model of polyurea using the Iterative Boltzmann Inversion (IBI) method. From equilibrium simulation of these CG models we have calculated the stress relaxation function of a linear polyurea with realistic molecular weights from which the frequency dependent storage and loss moduli can be computed. The predictions from these molecular simulations shed light on the dissipative properties of polyurea as well as elucidate trends in key chemical structure-property relationships. Additional coarse-grained models were created to study the effect of nano-inclusions with grafted polymer chains on the stress relaxation in polymer nanocomposites. At the continuum scale, the extended finite element method (XFEM) has been adapted to study the dissipative properties of inclusions within a polymer matrix. Furthermore, by considering interfaces that can fail in tension or shear loading, the feasibility of designing weak interfaces to further enhance energy dissipation has been studied.

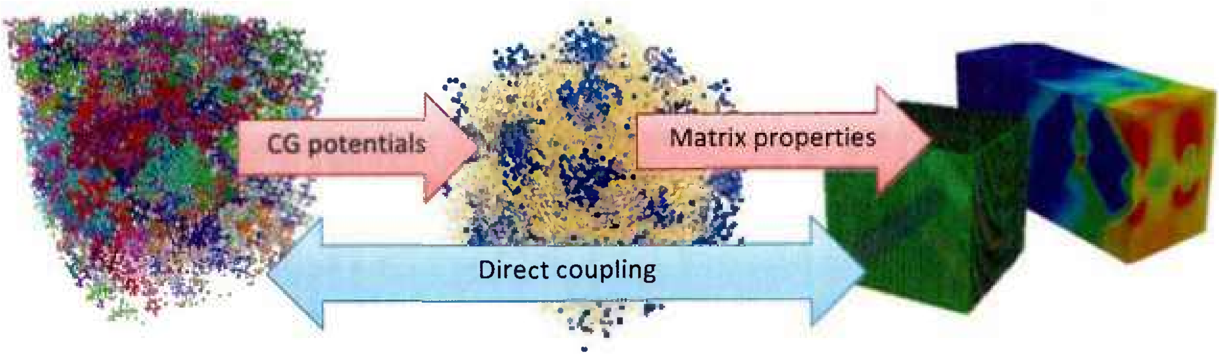

Figure 8: The three simulation scales, spanning from all-atom simulations, to coarse-grained molecular dynamics, to continuum mechanics of composite polyurea.

Reactive Molecular Dynamics Modeling by ReaxFF Potential

Classical molecular dynamics force fields such as the PCFF and COMPASS utilize simple polynomial relationships for bond and angle potentials as well as fixed partial charges within molecules. As a result, covalent bonds are not broken in these models, and as a result, these potentials cannot predict damage initiation for large strains. To better understand the behavior of polyurea at such strains, the ReaxFF potential, which enables chemical processes such as bond breakage and formation, as well as direct computation of partial charges through a simulation was used to model polyurea undergoing large deformation.

Figure 9 shows the progression of a periodic volume of polyurea being subjected to a biaxial extension. In each snapshot, atoms belonging to the hard segments are red, while atoms belonging to the soft flexible segments of polyurea are green. At large deformation, voids nucleate from within the soft flexible regions with fibril formation occurring between connected domains composed primarily of hard segments.

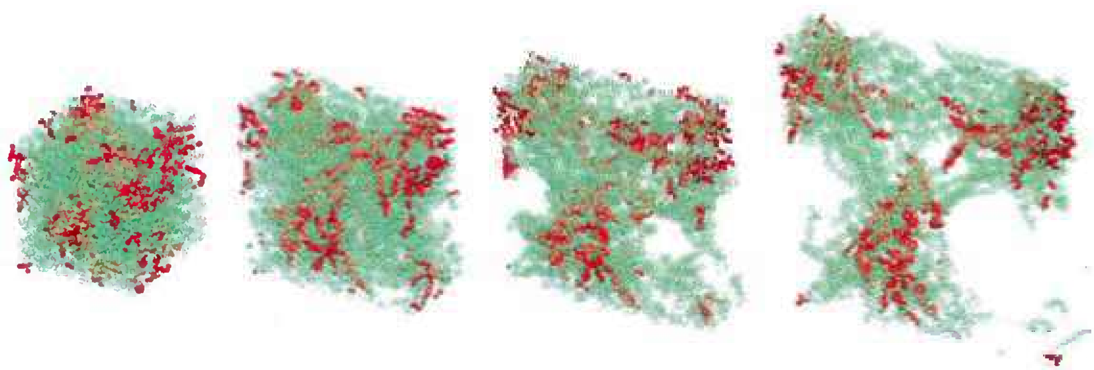

Figure 9: MD simulations with reactive force field of polyurea under biaxial loading showing damage evolution.

Validation of Coarse-Grained Model of Polyurea with the Benchmark Polyurea

A coarse-grained (CG) molecular dynamics model of polyurea, shown in Figure 10, is calibrated in a bottom up fashioned from atomistic molecular dynamics simulations and validated against experiments conducted on the controlled, benchmark polyurea material. The CG model matches the structural distributions generated by the atomistic model through effective potentials derived through the iterative Boltzmann inversion method.

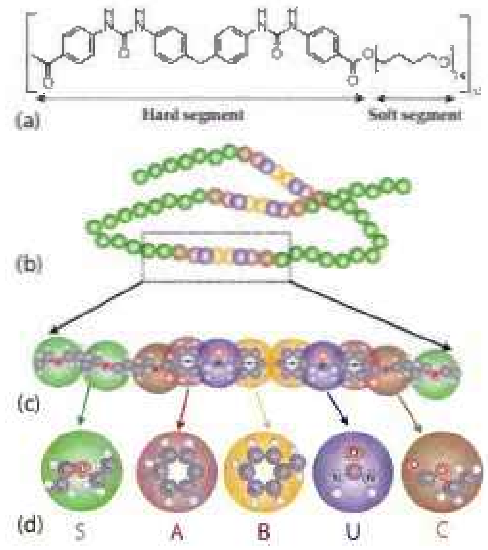

Figure 10 Coarse-grained model of polyurea: (a) chemical structure of the repeating units of polyurea consisting of alternating hard and soft segments, (b) figurative representation of a short polyurea chain composed of coarse-grained beads, (c) coarse-grained mapping of hard and soft segments of polyurea, and (d) chemical structure of coarse-grained bead types.

From equilibrium simulations conducted on the CG and fully atomistic models, the stress relaxation function is calculated from the autocorrelation of the virial stress and rescaled in time by a time-dependent dynamic scaling function calibrated to match the self-diffusion of the atomistic and coarse-grained models. Master curves computed from the stress relaxation function are then compared with dynamical mechanical analysis and ultrasonic testing of the benchmark material. Figure 11 shows the excellent agreement between the predicted and measured dynamic moduli of the benchmark polyurea.

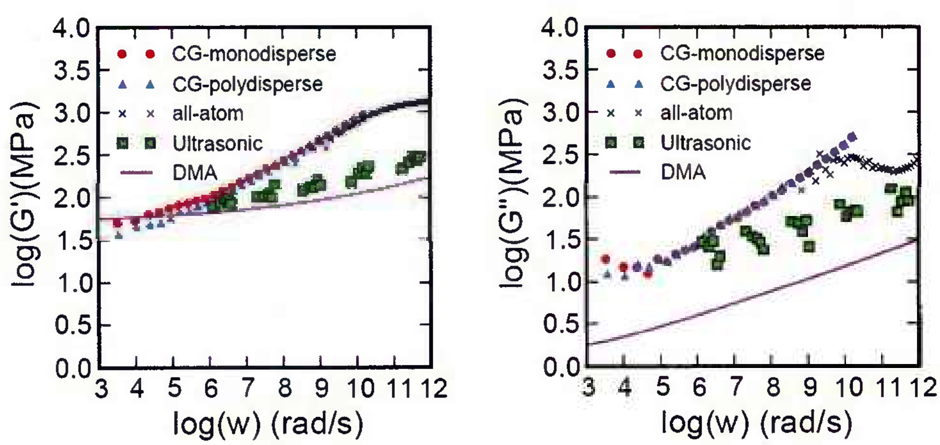

Figure 11: Comparison of frequency-dependent storage moduli and loss moduli obtained from CG simulation, all-atom MD simulation, and experimental results obtained from ultrasonic and DMA data.

Finite Element Modeling of Pressure/Shear Ball Impact Experiment

To simulate permanent deformation and damage to the polyurea specimens during the pressure-shear impact testing, a viscoelastic-plastic continuum damage model based on void growth was implemented within a 2D, axisymmetric finite element code. The viscous deformation of this model is governed by the pressure and temperature dependent relaxation function developed by Amirkhizi et al [1], and a viscoplastic damage model, based on Gurson's void growth model [2] are combined to represent the material response up to the point of failure. The pressure-shear impact test is conducted by firing a steel ball with a gas gun at a thin polyurea specimen behind which is a steel anvil with a spherical indent. As the polyurea is force into the indentation in the anvil, both extreme pressure and shear stresses are generated. Figure 12 shows a typical simulation result where the most porosity is observed to be generated along the radial centerline and around the edge of the contact between the ball and the specimen.

The key difference between the model as implemented for polyurea and Gurson's original model is the choice of the void nucleation rate. In Gurson's model void nucleation is generated through plastic strain, which initially is only generated though shear deformation. In this current model for polyurea, the void nucleation rate is controlled through the rate of hydrostatic stress

$$\dot{f}_{nucl} = \frac{f_N}{s\sigma_y\sqrt{2\pi}} \exp\left(-\frac{1}{2}\left(\frac{\Sigma_h - \sigma_N}{s\sigma_y} \right)^2 \right) \dot{\Sigma}_h$$

where f_N is the volume fraction of void nucleation sites, Σ_h is the hydrostatic part of the macroscopic stress tensor, s and σ_N control the standard deviation and mean value of the void growth distribution function, and σ_y is the shear yield stress of the material.

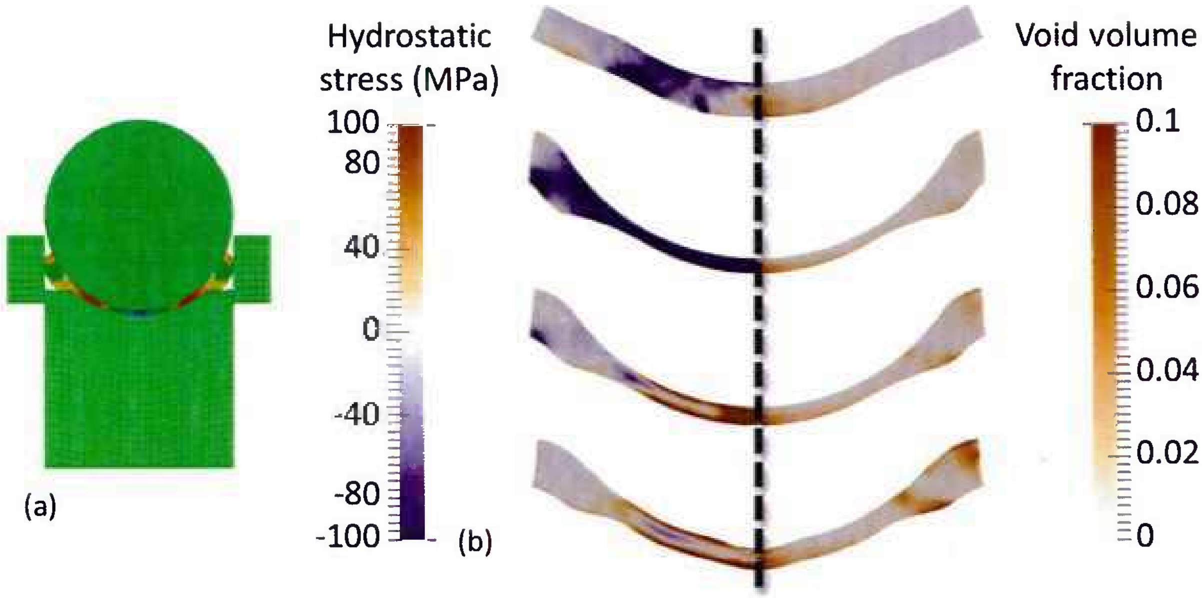

Figure 12: Finite element model of pressure shear impact experiment: a) snapshot of simulation when the polyurea specimen is under maximum compression, b) evolution of hydrostatic stress and void volume fraction within the highly deformed part of the specimen.

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[1] A. Amirkhizi, J. Isaacs, J. McGee, and S. Nemat-Nasser, "An experimentally-based viscoelastic constitutive model for polyurea, including pressure and temperature effects," *Phil. Magazine*, vol. 86, pp. 5847-5866, 2006.

[2] A. L. Gurson, "Continuum theory of ductile rupture by void nucleation and growth. Part I. Yield criteria and flow rules for porous ductile media," Brown Univ., Providence, RI (USA) Div. of Engineering, 1975.

UCSD/CEAM COLLABORATIONS AND INTERACTIONS

- NSWC Carderock Division [Phil Dudt and Alyssa Littlestone]
- MIT [Prof. Raul Radovitzky]
- University of Texas at Austin [Prof. K. Ravi-Chandar]
- California Institute of Technology [Prof.'s G. Ravichandran and W. Knauss, and Graduate Students Matthew Newman and Victoria Stolyar]
- NSWC Dahlgren Division [Bill Mock and Susan Bartyczak]
- University of Massachusetts, Lowell [Prof. Alireza Amirkhizi]

ARCHIVAL PUBLICATIONS, CONFERENCE PROCEEDINGS AND PRESENTATIONS

I. Archival Journals [Published and In-Press]

[1] Qiao, J., A.V. Amirkhizi, K. Schaaf and S. Nemat-Nasser, "Dynamic Mechanical Analysis of Fly Ash Filed Polyurea Elastomer," *J. Eng. Moter. Technol.*, Special Issue, Vol. 133, No. 1 (2011) 011016, 7 pages.

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II. CONFERENCE PROCEEDINGS

Qiao, J., K. Schaaf, A.V. Amirkhizi and S. Nemat-Nasser, "Effect of Particle Size and Volume Fraction on Tensile Properties of Fly Ash/Polyurea Composites, *Proceedings of Electroactive Polymer Actuators and Devices (EAPAD) 2010,* SPIE's 17th Annual International Conference on Smart Structures and Materials, San Diego, CA, March 2010 (2010).

Amirkhizi, A.V., J. Qiao, K. Schaaf and S. Nemat-Nasser, "Properties of Elastomer-based Particulate Composites," *Proceedings SEM Annual Conference and Exposition on Experimental and Applied Mechanics*, Indianapolis, IN, June 2010 ISBN: 978-1-935116-05-9 (2010) 4 pages. [Extended Abstract].

Amirkhizi, A.V., J. Qiao, W. Nantasetphong, K. Schaaf and S. Nemat-Nasser, "Experimental Investigation of Dynamic Mechanical Properties of Polyurea-Fly Ash Composites" *Proceedings of SEM Annual Conference and Exposition on Experimental and Applied Mechanics,* Uncasville, CT, June 2011, (2011) 2 pages. [Extended Abstract].

Schaaf, K. and S. Nemat-Nasser, "Characterization of Elastomeric Composite Materials for Blast Mitigation," *Proceedings SEM Annual Conference and Exposition on Experimental and Applied Mechanics,* Uncasville, CT, June 2011, (2011) 3 pages. [Extended Abstract].

Schaaf, K. and S. Nemat-Nasser, "Blast Resistant Elastomeric Polymer-by-Design," *Proceedings from ASME 2011 International Mechanical Engineering Congress & Exposition,* Denver, CO, November 2011, (2011) 2 pages. [Extended Abstract].

Nantasetphong, W., A. V. Amirkhizi, Z. Jia and S. Nemat-Nasser, "Polyurea-based Composites: Ultrasonic Testing and Dynamic Mechanical Properties Modeling" *2012 Annual SEM Conference,* Costa Mesa, CA, June 2012, (2012) 8 pages.

Song, Y., J. Isaacs, R. Griswold, A. Srivastava, A. V. Amirkhizi and S. Nemat-Nasser, "Shock Wave Interaction with Periodic Obstacles," *2012 Annual SEM Conference*, Costa Mesa, CA, June 2012, (2012) 5 pages.

Jia, Z., K. Holzworth and S. Nemat-Nasser, "Milled Glass Reinforced Polyurea Composites: The Effect of Surface Treatment," *2012 Annual SEM Conference*, Costa Mesa, CA, June 2012, (2012) 3 pages. [Extended Abstract].

Holzworth, K., G. Williams and S. Nemat-Nasser, "Hybrid Polymer Grafted Nanoparticle Composites for Blast-induced Shock-wave Mitigation," *2012 Annual SEM Conference*, Costa Mesa, CA, June 2012, (2012) 2pages. [Extended Abstract].

Holzworth, K., G. Williams, B. Arman, Z. Guan, G. Arya and S. Nemat-Nasser, "Polyurea with Hybrid Polymer Grafted Nanoparticles: A Parametric Study," *Proceedings of the ASME 2012 IMECE*, Nov. 9-15 2012, Houston TX. (2012) 2 pages. [Extended Abstract].

Qiao, J., A.V. Amirkhizi, S. Nemat-Nasser, G. Wu, "Ultrasonic Studies of Fly Ash/Polyurea Composites," *Proceedings of 2013 SPIE Annual Conference, Behavior and Mechanics of Multifunctional Materials and Composites,* Vol. 8689, (2013) 86891C-1-5, (2013) 5 pages.

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Nantasetphong, W., A.V. Amirkhizi, Z. Jia and S. Nemat-Nasser, "Low-Density, Polyurea-Based Composites: Dynamic Mechanical Properties and Pressure Effect," *Challenges In Mechanics of Time-Dependent Materials and Processes in Conventional and Multifunctional Materials*, Vol. 2, Chp. 16 (2014) 145-150, Proc. of 2013 SEM Conference, Chicago, Il, SEM Series, DOI 10.1007/978-3-319-00852-3_16.

Jia, Z., A. V. Amirkhizi, K. Holzworth and S. Nemat-Nasser, "The Effect of Stoichiometric Ratio on Viscoelastic Properties of Polyurea," *Challenges In Mechanics of Time-Dependent Materials and Processes in Conventional and Multifunctional Materials*, Vol. 2, Chp. 3 (2014) 17 – 20, Proc. of 2013 SEM Conference, Chicago, IL, SEM Series, DOI 10.1007/978-3-319-00852-3_3.

Jia, Z, J. Isaacs, R. Rawal and S. Nemat-Nasser, "Tailored Polyurea-Glass Interfaces and the Characterization by The Single-Fiber Fragmentation," *Proc. of ASME 2013 International Mechanical Engineering Congress & Exposition,* San Diego, CA, Nov. 2013, IMECE2013-63736 (2013) 2 pg. [Extended Abstract].

Qiao, J., A.V. Amirkhizi and S. Nemat-Nasser, "Effect of Particle Size on the Properties of Polyurea-Based Composites," *Proc. of SPIE Smart Structures NDE 2015, Behavior and Mechanics of Multifunctional Materials and Composites IX*, edited by M. Goulbourne, Vol. 9432, 94320R (2015) 5pp.

Jia, Z., A.V. Amirkhizi, W. Nantasetphong and S. Nemat-Nasser, "Determining the Shear Relation Modulus and Constitutive Models for Polyurea and Polyurea-based Composite Materials from Dynamic Mechanical Testing Data," *Springer Proceedings SEM 2015*, June 2015 (2015) 5pp.

III. PRESENTATIONS AT CONFERENCES/SYMPOSIA/WORKSHOPS

"Acoustic and Ultrasonic Properties of Pressure-sensitive Elastomers," A.V. Amirkhizi, J. Qiao and S. Nemat-Nasser, ASME IMECE, Symposium on Mechanics of Solids, Structures and Fluids: top-Down and Bottom-Up Approaches to Fracture, FL, Nov. (2009).

"Effect of Particle Size and Volume Fraction on Tensile Properties of Fly Ash/Polyurea Composites" J. Qiao, K. Schaaf, A.V. Amirkhizi, S. Nemat-Nasser, SPIE's 17th Annual International Conference on Smart Structures and Materials, San Diego, CA, Mar. (2010).

"Properties of Elastomer-based Particulate Composites," A.V. Amirkhizi, J. Qiao, K. Schaaf and S. Nemat-Nasser, SEM Annual Conference and Exposition on Experimental and Applied Mechanics, Indianapolis, IN, June (2010).

"Elastomeric Composite Materials for Shock Mitigation," K. Schaaf and S. Nemat-Nasser, SPIE's 18th Annual International Conference on Smart Structures and Materials, San Diego, CA, Mar. (2011).

"Characterization of Elastomeric Composite Materials for Blast Mitigation," K. Schaaf and S. Nemat-Nasser, SEM Annual Conference and Exposition on Experimental and Applied Mechanics, Uncasville, CT, June (2011).

"Experimental Investigation of Dynamic Mechanical Properties of Polyurea-Fly Ash Composites", A. V. Amirkhizi, J. Qiao, W. Nantasetphong, K. Schaaf, S. Nemat-Nasser, SEM Annual Conference and Exposition on Experimental and Applied Mechanics, Uncasville, CT, June (2011).

"Modeling of Elastomeric Polymers for Blast-Induced Shock Wave Management," J. Oswald, D. O'Connor, Z. Liu, and T. Belytschko, 11th U.S. National Congress on Computational Mechanics, July 25, (2011).

"XFEM modeling of ultrasonic wave propagation in particulate/fibrous polymer matrix composite," Z. Liu, J. Oswald, and T. Belytschko, 11th U.S. National Congress on Computational Mechanics, July 25, (2011).

"Modeling of Titin" [Poster Presentation], Yesuk Song and Sia Nemat-Nasser, US Korea Conference on Science, Technology and Entrepreneurship, Park City, UTAH, Aug.11-12, (2011).

"Coarse graining for soft materials in LAMMPS," J. Oswald, LAMMPS Users' Workshop, Albuquerque, NM, Aug., (2011).

"Multiscale Modeling Of Elastomeric Polymers For Blast-induced Shock Wave Management", J. Oswald, D. O'Connor, T. Belytschko, 48th Annual Technical Conference of Society of Engineering Science (SES), Evanston, IL, Oct. 12-14, (2011).

"XFEM Modeling Of Ultrasonic Wave Propagation In Polymer Matrix Particulate/fibrous Composites" Z. Liu, J. Oswald, T. Belytschko, 48th Annual Technical Conference of Society of Engineering Science (SES), Evanston, IL, Oct. 12-14, (2011).

"Adaptive Atomistic-to-Continuum Modeling of Propagating Defects," P. Moseley, J. Oswald and T. Belytschko, 48th Annual Technical Conference of Society of Engineering Sciences (SES), Evanston IL, Oct.12-14, (2011).

"Blast Resistant Elastomeric Polymer-by-Design," K. Schaaf and S. Nemat-Nasser, ASME 2011 International Mechanical Engineering Congress & Exhibition, Denver, CO, Nov. (2011). *[Invited Presentation]*

"The Effect of Microstructural Heterogeneity on Dynamic Properties of Polyurea", A. V. Amirkhizi, J. Qiao, S. Nemat-Nasser, ASME 2011 International Mechanical Engineering Congress& Exhibition, Denver, CO, Nov. (2011) *[Invited Presentotion]*

"Nanoparticle superlattice for blast-induced shock-wave management," K. Holzworth, G. Williams, S. Nemat-Nasser, 2012 SPIE Smart Structures and Materials & Nondestructive Evaluation and Health Monitoring, San Diego, CA, Mar. 11-15, 2012

"Milled Glass Reinforced Polyurea Composites: the Effect of Surface Treatment," Z. Jia, K. Holzworth, and S. Nemat-Nasser, 2012 SEM Annual Conference, Costa Mesa CA, June 10-14, 2012

"Polyurea-based Composites: Ultrasonic Testing and Dynamic Mechanical Properties Modeling," W. Nantasetphong, A.V. Amirkhizi, Z. Jia and S. Nemat-Nasser, 2012 SEM Annual Conference, Costa Mesa CA, June 10-14, 2012

"Hybrid Polymer Grafted Nanoparticle Composites for Blast-Induced Shock-Wave Management," K. Holzworth, G. Williams and S. Nemat-Nasser, 2012 SEM Annual Conference, Costa Mesa CA, June 10-14, 2012.

"Shock wave Interaction with Periodic Obstacles," Y. Song, J. Isaacs, R. Griswold, A. Srivastava, A. V. Amirkhizi, S. Nemat-Nasser, 2012 SEM Annual Conference, Costa Mesa CA, June 10-14, 2012.

"Interaction of a Shock-Wave with Elastically Constrained Periodic Obstacles: Estimated and Visualization" S. Nemat-Nasser and Y. Song [Invited Talk], ASME International Mechanical Engineering Congress and Exposition, Houston TX, Nov. 9-1S 2012.

"Polyurea with Hybrid Polymer Grafted Nanoparticles: A Parametric Study," Holzworth, K., G. Williams, B. Arman, Z. Guan, G. Arya and S. Nemat-Nasser, ASME International Mechanical Engineering Congress and Exposition, Houston, TX, Nov. 9-15 2012.

"Coarse-grained and all-atom modeling of polyurea composites for shock wave dissipation," J. Oswald, P. Moseley, and T. Belytschko, ASME Intl. Mechanical Engineering Congress and Exposition, Houston, TX, Nov. 9-1S 2012.

"Effect of chain architecture on the viscoelasticity and shock response of block copolymers" B. Arman, A. Srinivas Reddy, and G. Arya, 2012 AIChE Meeting, Pittsburgh, PA, Nov. 2012.

"Ultrasonic studies of fly ash/polyurea composites," J. Qiao, A.V. Amirkhizi, S. Nemat-Nasser, G. Wu, SPIE 2013 Annual Conference, San Diego, CA, Mar. 2013.

"Modifying the Acoustic Impedance of Polyurea-based Composites," W. Nantasetphong, A.V. Amirkhizi, A. Jia and S. Nemat-Nasser, SPIE 2013 Annual Conference, San Diego, CA, Mar.2013.

"Low-Density, Polyurea-Based Composites: Dynamic Mechanical Properties and Pressure Effect," W. Nantasetphong, A.V. Amirkhizi, Z. Jia and S. Nemat-Nasser, *Chollenges In Mechonics of Time-Dependent Moteriols ond Processes in Conventionol ond Multifunctionol Moteriols*, 2013 SEM Conference, Chicago, June 2013.

"The Effect of Stoichiometric Ratio on Viscoelastic Properties of Polyurea," Z. Jia, A. V. Amirkhizi, K. Holzworth and S. Nemat-Nasser, *Chollenges In Mechonics af Time-Dependent Materiols ond Processes in Conventionol ond Multifunctional Materials*, 2013 SEM Conference, Chicago, IL June 2013.

"A coarse-grained representation of polyurea for modeling wave dissipation due to blast loading," V. Agrawal, G. Hattemer, G. Arya, J. Oswald, 12th U.S. Natl. Congress on Computational Mechanics (USNCCM12), Raleigh, NC, July 2013.

"3D Modeling of Fiber Reinforced Polyurea Composite Materials Under Impact Loading," J. Zhao, J. Oswald, T. Belytschko, 12th U.S. National Congress on Computational Mechanics (USNCCM12), Raleigh, NC, July 2013.

"A Genetic Algorithm for Efficient Numerical Integration of Nodal Forces in Extended Finite Element Simulations," X. Liao, J. Oswald, 12th U.S. National Congress on Computational Mechanics (USNCCM12), Raleigh, NC, July 2013.

"Viscoelastic behavior of grafted-nanoparticle/polymer composites," G. Hattemer and G. Arya, 2013 American Institute of Chemical Engineers (AIChE) Annual Meeting, San Francisco, CA, November 2013.

"Tailored Polyurea-Glass Interfaces and the Characterization by the Single-fiber Fragmentation," Z. Jia, J. Isaacs, S. Nemat-Nasser, ASME Intl. Mechanical Engineering Congress and Exposition, San Diego, CA, Nov. 18-21, 2013.

"Cross-linked Superlattice Nanocomposites for Shock-Wave Management," K. Holzworth, O. Cromwell, G. Williams, Z. Guan, S. Nemat-Nasser, ASME Intl. Mechanical Engineering Congress and Exposition, San Diego, CA, Nov. 2013.

"Viscoelastic Properties of Polyurea under Pressure," W. Nantasetphong, A. Amirkhizi, and S. Nemat-Nasser, ASME International Mechanical Engineering Congress and Exposition, San Diego, CA, Nov. 18-21, 2013.

"The Magic of Deciphering High Strain-Rate and High-Pressure Properties of Elastomeric Composites, Using Low Frequency Measurements," S. Nemat-Nasser, TMS 2014, San Diego, CA February 16-20, 2014.

"Development of Time-domain Master Curves Using the Data of Dynamic Mechanical Analysis for Polyurea and Polyurea-based Composites, " Z. Jia, Alireza V. Amirkhizi and S. Nemat-Nasser, 2014 Smart Structures/NDE SPIE Conference, San Diego, CA March 9-13, 2014

"Benchmark Polyurea: Tuning Computational Tools" K. Holzworth, Z. Jia, A. Amirkhizi and S. Nemat-Nasser, SEM 2014 Annual Conference & Exposition on Experimental and Applied Mechanics, Greenville, SC, June 2-5, 2014.

"Advanced Materials: The Magic of Deciphering Special Properties of Elastomeric Composites" S. Nemat-Nasser, UCSD Osler Lifelong Learning Institute - Distinguished Lecture, La Jolla, CA August 4, 2014.

"Advanced Materials: The Magic of Deciphering Special Properties of Elastomeric Composites" S. Nemat-Nasser, Penn State, *Material Science & Engineering Departmental Seminar - Distinguished Lecture*, State College, PA Sept. 24-26, 2014.

"Prediction and Validation of Viscoelastic Properties of Polyurea with Systematically Coarse-Grained Molecular Dynamics," J. Oswald, V. Agrawal, K. Holzworth, W. Nantasetphong, A. V. Amirkhizi, and S. Nemat-Nasser, MMM2014, Berkeley CA October 2014.

"The Magic of Deciphering High Strain-Rate and High-Pressure Properties of Elastomeric Composites Using Low Frequency Measurements, " S. Nemat-Nasser, IMECE 2014, Drucker Symposium, Montreal, CN November 14-20. 2014.

"Effect of Particle Size on the Properties of Polyurea-Based Composites," J. Qiao, A.V. Amirkhizi and S. Nemat-Nasser, SPIE Smart Structures NDE 2015, Behavior and Mechanics of Multifunctional Materials and Composites IX, San Diego, CA March 2015.

"Determining the Shear Relation Modulus and Constitutive Models for Polyurea and Polyurea-based Composite Materials from Dynamic Mechanical Testing Data, " Z. Jia, A.V. Amirkhizi, W. Nantasetphong and S. Nemat-Nasser, 2015 SEM Conference, Costa Mesa, CA June 8-11, 2015.

PHD DEGREES AWARDED/THESIS DISSERTATIONS

- Jing Qiao, Ph.D. Doctoral Degree in Engineering – Specialty Materials Science, August 2011, "Research on Viscoelastic Properties of Fly Ash/Polyurea Composites" Degree-Conferring Institution: Harbin Institute of Technology, China [S. Nemat-Nasser – Dissertation Committee Member and Research Mentor [at CEAM UCSD 9/30/08-8/31/10].
- Jay Oswald, Ph.D. Doctoral Degree in Mechanical Engineering, August 2011. Thesis Title: "An Extended Finite Element Method for Dislocations in Arbitrary Three-Dimensional Entities," Advisor: Ted Belytschko, NWU [Partially Supported].
- Phil Moseley, Ph.D. Doctoral Degree in Mechanical Engineering, August 2012. Thesis Title: "Multiscale Atomistic-Continuum Modeling of Complex Behavior" Advisor: Ted Belytschko, NWU.
- Greg Williams, Ph.D. Doctoral Degree in Chemistry, January 2013. Thesis Title: " Synthesis and Investigation of Dynamically Assembled Nanomaterials Using Supramolecular Interactions" Advisor: Zhibin Guan, UC Irvine.
- Olivia Cromwell, Ph.D. Doctoral Degree in Chemistry, June 2015. Thesis Title: "Synthesis and Investigation of Biomimetic Materials Employing Dynamic Interactions" Zhibin Guan, UC Irvine.

SCIENTIFIC PERSONNEL – RESEARCH FOCUS

UC San Diego

PI: Prof. Sia Nemat-Nasser – Mechanical and Aerospace Engineering/CEAM
Prof. Yitzhak Tor – Chemistry and Biochemistry
Prof. Gaurav Arya - Nanoengineering

Alireza Vakil Amirkhizi – Assistant Research Scientist – CEAM - Physical modeling of polyurea and polyurea-based particulate composites and their high-frequency testing and high-pressure testing.

Kristin Holzworth – Postdoctoral Researcher/Assistant Project Scientist – CEAM - Characterization of hybrid polymer grafted nanoparticle reinforced polyurea composites; NSWCCD/MIT and UT Austin collaboration liaison/researcher.

Christian Nielsen – Postdoctoral Researcher – CEAM – Development of experimental techniques for impact induced high-rate shearing under high pressure [partial support].

Zhanzhan Jia - PhD Student/Research Assistant – CEAM - Fabrication and characterization of milled glass reinforced polyurea composites and the effect of surface treatments, development of master curves for polyurea chemical variations and composites.

Yesuk Song - PhD Student/Research Assistant – CEAM - Development of Schlieren imaging experimental setup for shock-wave visualization, characterization of interaction of shock-waves with materials. Characterization of polyurea and polyurea-based composites at very high pressures using diamond anvil cell coupled with atomic force microscopy to study change in mechanical properties associated [partial support]

Wiroj Nantasetphong - PhD Student/Research Assistant – CEAM - Micro-mechanical modeling and experimental characterization of polyurea-based particulate composites. [Partial support].

Greg Hattemer – Staff Research Associate – Nanoengineering – Development of coarse-grained models of polyurea nanocomposites and molecular dynamics simulations to investigate the viscoelastic properties of the nanocomposites.

Bedri Arman –Postdoctoral Researcher – Nanoengineering - Development and mechanical calculations of coarse-grained models of polymers.

Renatus Sinkeldam – Postdoctoral Researcher – Chemistry/Biochemistry - Interfacial chemistry characterization and development of robust synthesis motifs for bulk material with ordered, homogenously dispersed nanoparticles.

UC Irvine

Co-PI: Prof. Zhibin Guan - Chemistry and Biomedical Engineering

Olivia Cromwell - PhD Student/Research Assistant – UCI – Development, synthesis, and characterization of superlattices nanocomposites.

Aaron Kushner – Postdoctoral Researcher – UCI Development, synthesis, and characterization of benchmark polyurea for utilization in tuning computational tools.

Greg Williams – PhD Student/Research Assistant – UCI Development, synthesis, and characterization of hybrid polymer grafted nanoparticle composites and superlattice nanocomposites.

Northwestern University

Co-PI: Prof. Ted Belytschko (Co-PI) –Mechanical Engineering
Prof. Wing Kam Liu

Jay Oswald - PhD Student/Research Assistant /Postdoctoral Researcher – Atomistic simulations of long chain molecules.

Jifeng Zhao – PhD Student/Research Assistant– Extended finite element simulations of energy dissipation through debonding of weak matrix-particle interfaces. XFEM modeling of weak interfaces.

Zhanli Liu - Postdoctoral Researcher –finite element analysis of wave propagation in highly heterogeneous media using XFEM.

Arizona State University

Prof. Jay Oswald – (as of August 2011) – ASU - Atomistic simulations of long chain molecules & production of fully calibrated CG potentials.

Vipin Agrawal – PhD Student/Research Assistant – ASU - Modeling the effect of polyurea chemistry and chain structure on stress relaxation with coarse-grained molecular dynamics and validation of coarse-grained model of polyurea with the benchmark polyurea.

Xiao Liao - PhD Student/Research Assistant – ASU - Development of extended finite element methods for dynamical simulation of complex microstructures. Continuum damage modeling and finite element modeling of impact induced high-rate shearing under high pressure.

VITAL STATISTICS

Number of Conferred PhD's: 5
Number of Conferred Masters Degrees: 0
Number of Graduate Students: 16 (3 female, 0 minority)
Number of Undergraduate Student Researchers: 2 (1 female, 0 minority)
Number of Publications and Reports: 11 [Archival]

Elastomeric Polymer-by-Design for Blast-Induced Shock-Wave Management

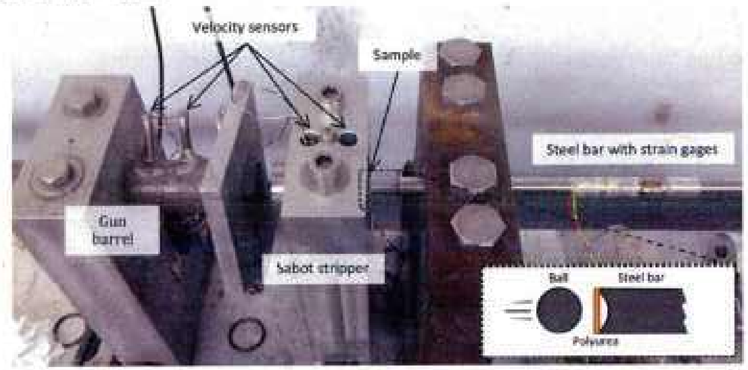
Sia Nemat-Nasser, UC San Diego

Grant: N00014-09-1-1126

S&T OBJECTIVES

- To develop innovative experimental techniques and corresponding computational simulations to characterize polyurea at extreme conditions

EXAMPLE



The experimental setup for producing combined high pressure and shear in polymer samples. The incident ball bearing exits the gas gun barrel (left), passes through a sabot stripper (center left), and impacts the polyurea sample (center) sitting at the end of a steel bar (right).

APPROACH

Experimental Efforts

- Mild Pressure
  - Ultrasonic measurements using a low pressure cell
- High Pressure
  - Ultrasonic measurements using a high pressure cell
  - Impact-induced high-rate shearing under high pressure
- Very High Pressure
  - Optical spectroscopy using a diamond anvil cell (DAC)

Computational Efforts

- Reactive Molecular Dynamics Modeling by ReaxFF Potential
- Validation of Coarse-Grained Model of Polyurea with the Benchmark Polyurea
- Finite Element Modeling of Pressure/Shear Ball Impact Experiment

RESULTS and ONGOING RESEARCH

- Designed and constructed an experimental facility to subject polyurea to combined high pressure and shear at high strain rates
- Developed compressive-mode confinement cells for ultrasonic wave measurement characterization of polyurea at high pressure
- Observed behavior of polyurea at very high pressure over 3 GPa using diamond anvil cell
- Used ReaxFF potential, which enables chemical processes, to model polyurea undergoing large deformation
- Developed a coarse-grained molecular dynamics model of polyurea and validated against experiments of benchmark polyurea material
- Simulated pressure-shear experiment using 2D, axisymmetric finite element model